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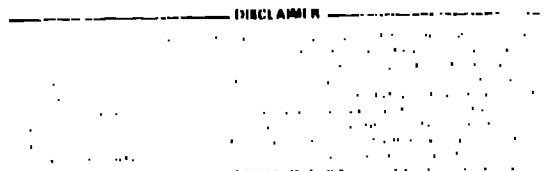
TITLE: SENSIT:
A CROSS-SECTION AND DESIGN SENSITIVITY AND UNCERTAINTY
ANALYSIS CODE

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SUBMITTED TO: For presentation to the Specialists' Meeting on
Nuclear Data and Benchmarks for Reactor Shielding,
and for inclusion into the meeting's proceedings
in Paris, France

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SENSIT: A CROSS-SECTION AND DESIGN SENSITIVITY
AND UNCERTAINTY ANALYSIS CODE

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ABSTRACT

SENSIT computes the sensitivity and uncertainty of a calculated integral response (such as a dose rate) due to input cross-sections and their uncertainties. Sensitivity profiles are computed for neutron and gamma-ray reaction cross-sections of standard multigroup cross-section sets and for secondary energy distributions (SED's) of multigroup scattering matrices. In the design sensitivity mode, SENSIT computes changes in an integral response due to design changes and gives the appropriate sensitivity coefficients. Cross-section uncertainty analyses are performed for three types of input data uncertainties: (a) cross-section covariance matrices for pairs of multigroup reaction cross-sections, (b) spectral shape uncertainty parameters for secondary energy distributions (integral SED uncertainties), and (c) covariance matrices for energy-dependent response functions. For all three types of data uncertainties SENSIT computes the resulting variance and estimated standard deviation in an integral response of interest, based on generalized perturbation theory. SENSIT attempts to be more comprehensive than earlier sensitivity analysis codes, such as SWANLAK.

Introduction

Sensitivity analysis in radiation transport theory attempts to determine quantitatively how sensitive a calculated integral response is to the input data for the transport calculation. Such input data may concern either cross-section data, geometry specifications (design data), methods approximations, or any other input required to perform a transport calculation. In an uncertainty analysis, the sensitivity information is used, together with additional data about the uncertainty of the input data, to calculate or estimate the uncertainty of a calculated integral response which results from these input data uncertainties. In a cross-section uncertainty analysis the data uncertainties may be quantified in cross-section covariance matrices and in spectral shape uncertainty parameters for secondary energy distributions (SED's), while the resulting response uncertainty is best quantified by a variance or relative standard deviation. In a design sensitivity analysis, usually a specific design change, e.g. a material replacement or a geometry modification, and its effect on a calculated integral response is of concern. Therefore, in such cases a resulting response change is calculated based on generalized perturbation theory.

The SENSIT code is in some respects more comprehensive than earlier sensitivity codes presently in use [1]. Specifically, SENSIT includes the calculation of sensitivity profiles for secondary energy distributions (SED's) and performs also an SED uncertainty analysis. In addition, SENSIT also allows design sensitivity analyses and detector response uncertainty analyses to be performed in addition to the standard cross-section sensitivity and uncertainty analysis.

Detailed documentation on SENSIT is published separately in a comprehensive Los Alamos Scientific Laboratory Report, Ref. [2]. This 128-pages report contains detailed descriptions of the SENSIT input specifications, the underlying theory, the computational outline, details of program options, eight sample problems, retrieving and running SENSIT on two different CDC-7600 computers, references, and listings of all sample problems' input and output files. A separate Los Alamos Scientific Laboratory report, Ref. [3], documents in detail the application of SENSIT to a comprehensive neutron cross-section and secondary-energy-distribution uncertainty analysis for a fusion reactor. Due to the availability of this detailed documentation in the open literature, we restrict ourselves in the following to a summary of the significant features of SENSIT.

Computer Code Abstract

1. Program Identification: SENSIT
2. Computer for which program is designed: CDC-7600, IBM 360
3. Description of Function and Method of Solution:

The basic theory upon which the present sensitivity and uncertainty analysis methods are based has developed over the past several years. We refer to only a few selected references here which can provide the user an overview of the field, Refs. [4] through [7]. More mathematical detail is given in Ref. [8] with special emphasis on discrete-ordinates formulations. SENSIT is based on the one-dimensional discrete-ordinates formulation of radiation transport theory and operates in four different modes which can be selected by setting an input parameter ITYP to an integer value between zero and three as indicated below:

- A. Standard Cross-Section Sensitivity Analysis (ITYP = 0)

Conventional sensitivity profiles P_i may be derived from the expression for the forward difference approximation, Eq. (36) in Ref. [8], or Eq. (17) in Ref. [4], or Eq. (26) in Ref. [5]. The analytical definition of a cross-section sensitivity function $F_{i,x}(E)$ expresses the sensitivity of a calculated integral response I to a particular cross section $\Sigma_{x,i}$ at energy E and may be expressed as

$$F_{i,x}(E) = (1/I) \int d\mathbf{r} \int d\Omega \left\{ -\phi(\mathbf{r}, \Omega, E) \Sigma_{x,i}(\mathbf{r}, E) \phi(\mathbf{r}, \Omega, E) \right. \\ \left. + \int d\Omega' \int dE' \phi(\mathbf{r}, \Omega, E) \Sigma_{x,i}(\mathbf{r}, \Omega' E', E+E') \phi(\mathbf{r}, \Omega', E') \right\} \quad (1)$$

In a multigroup formulation one usually prefers to identify and work with a sensitivity profile P_{Σ}^g , which is related to the above sensitivity function through the scaling factor Δu^g by $P_{\Sigma}^g = \bar{F}_{\Sigma}(E_g)/\Delta u^g$, and refers to a group-averaged sensitivity. Δu^g is the lethargy width of energy group g . The exact numerical definition of a multigroup cross-section sensitivity profile for the macroscopic cross section Σ_x^g is:

$$P_{\Sigma_x}^g = \left\{ -\Sigma_{x,T}^g \cdot \chi^g + \sum_{l=0}^{LMAX} \sum_{g'=g}^{GMAX} \Sigma_{s,l}^{g \rightarrow g'} \cdot \psi_l^{g \rightarrow g'} \right\} / I_{\phi} \Delta u^g, \quad (2)$$

where $\Sigma_{x,T}^g$ = total macroscopic cross section for reaction type x ,

$\Sigma_{s,l}^{g \rightarrow g'}$ = l 'th Legendre coefficient of the scattering matrix element for energy transfer from group g to group g' , as derived from the differential scattering cross section for reaction type x ,

$$\chi^g = \sum_{i=1}^{IPERT} V_i \sum_{m=1}^{MM} \phi_m^g(i) \cdot \phi_m^{*g}(i) \cdot \omega_m,$$

= numerical integral of the product of forward and adjoint angular fluxes over all angles and all spatial intervals described by $i = 1, \dots, IPERT$.

$$\psi_l^{g \rightarrow g'} = \sum_{i=1}^{IPERT} V_i X_l^g(i) \cdot Y_l^{g'}(i),$$

= spatial integral of the product of Legendre coefficients of forward and adjoint angular fluxes.

$$X_l^g(i) = \sum_{m=1}^{MM} \phi_m^g(i) \cdot P_l(\mu_m) \cdot \omega_m$$

$$Y_l^{g'}(i) = \sum_{m=1}^{MM} \phi_m^{*g'}(i) \cdot P_l(\mu_m) \cdot \omega_m$$

$\phi_m^g(i), \phi_m^{*g'}(i)$ = discrete-ordinates representations of forward and adjoint angular fluxes for group g , spatial mesh point i and discrete direction m .

$P_l(\mu_m)$ = Legendre polynomial of order l at direction cosine μ_m .

$[\mu_m, \omega_m]$ = discrete-ordinates quadrature direction cosines μ_m and associated quadrature weights ω_m .

V_i = volume of spatial mesh interval i .

Δu^g = lethargy width of energy group g , $\ln(E_g^u/E_g^l)$, where E_g^u and E_g^l are upper and lower energy group boundaries.

I_ϕ = integral response as calculated from forward fluxes only,

$$= \sum_{i=1}^{IDET} \sum_{g=1}^{IGM} \sum_{m=1}^{MM} V_i R_i^g \cdot \phi_m^g(i) \cdot w_m$$

R_i^g = spatially and group-dependent detector response function.

The basic Eq. (2), as well as its corresponding Eq. (1), consist of two terms on the right-hand side. The first term, which is always negative, is called the "loss term" [4,8] and involves always the total (collision) cross section for a certain reaction type. The second term involves only the differential scattering cross section and is always positive; it is called the "gain term" [4,8]. In order to facilitate the interpretation of sensitivity results, SENSIT prints loss and gain terms in addition to the net sensitivity profiles.

B. Design Sensitivity Analysis (ITYP = 1)

The objective in a design-sensitivity analysis is to estimate the change of an integral response I due to a given design change without repeating the transport calculation for the altered design. Methods, based on generalized perturbation theory, have been developed which allow such estimates to be made with second-order accuracy in respect to the associated flux changes [5,8]. These perturbation methods require only the forward and adjoint flux solutions to a reference case and the specification of a perturbation to this reference design, which is equivalent to a postulated design change. All such design changes can be described then by a perturbation, ΔL , in the linear Boltzmann operator L .

Due to the dualism of forward and adjoint formulations for radiation transport calculations, two different but equivalent expressions can be derived for the estimated integral response in the perturbed system [5,8]. These expressions are both second-order with respect to flux changes but first-order with respect to the perturbation and are denoted as the adjoint difference (AD) and the forward difference (FD) formulation. Using the convenient operator notation of Refs. [5] and [8], we obtain for the integral response in the perturbed system the two expressions

$$I_{AD}^{(2)} = \langle R, \phi \rangle + \langle \phi, \Delta L \phi \rangle, \quad I_\phi^{(1)} + \Delta I_{AD}^{(2)}, \quad (3)$$

$$I_{FD}^{(2)} = \langle Q, \phi \rangle + \langle \phi, \Delta L \phi \rangle, \quad I_\phi^{(1)} + \Delta I_{FD}^{(2)}, \quad (4)$$

where $\langle \cdot, \cdot \rangle$ indicates integrations over all independent variables, and ϕ , ϕ^* are the forward and adjoint angular fluxes for the reference design. If the operators ΔL and ΔL^* are written down explicitly [8], it is noted that the second-order term in Eq. (4) is equivalent to the negative of the numerator of Eq. (2) when the cross sections Σ_i are replaced by cross-section changes $\Delta \Sigma_i$, and when an additional integration over all energies E , namely, a summation over all groups g , is performed:

$$\Delta I_{FD}^{(2)} = \sum_{g=1}^{IGM} \left\{ \Delta \Sigma_T^g \cdot \phi^g - \sum_{s=1}^{IMAX} \sum_{v=g}^{IGM} \Delta \Sigma_{s,v}^g \cdot \phi_v^g \cdot \psi_v^g \right\}. \quad (5)$$

The analogous expression for the second-order term in Eq. (3) becomes

$$\Delta I_{AD}^{(2)} = \sum_{g=1}^{IGM} \left\{ \Delta \Sigma_T^g \cdot \phi^g - \sum_{s=1}^{IMAX} \sum_{v=g}^{IGM} \Delta \Sigma_{s,v}^g \cdot \phi_v^g \cdot \psi_v^g \right\}. \quad (6)$$

The perturbation, as expressed by macroscopic cross-section changes in Eqs. (5) and (6) is calculated in SENSIT from two sets of input cross-section tables, the unperturbed or reference cross-section set $\{\bar{Z}\}$ and the perturbed cross-section set $\{Z\}$:

$$\Delta \Sigma_T^R = \Sigma_T^R - \bar{\Sigma}_T^R, \quad (7)$$

$$\Delta \Sigma_{s,2}^{R \rightarrow R} = \Sigma_{s,2}^{R \rightarrow R} - \bar{\Sigma}_{s,2}^{R \rightarrow R} \quad (8)$$

$$\Delta \Sigma_{s,2}^{R \rightarrow \gamma} = \Sigma_{s,2}^{R \rightarrow \gamma} - \bar{\Sigma}_{s,2}^{R \rightarrow \gamma} \quad (9)$$

A design sensitivity coefficient X is then defined for both (AD and FD) formulations according to

$$X_{AD} = I_{AD}^{(2)} / I_{\phi}^{(1)} = 1 - \Delta I_{AD}^{(2)} / I_{\phi}^{(1)}, \quad (10)$$

$$X_{FD} = I_{FD}^{(2)} / I_{\phi^*}^{(1)} = 1 - \Delta I_{FD}^{(2)} / I_{\phi^*}^{(1)}, \quad (11)$$

from which the estimated fractional change of the integral response I due to the introduction of the perturbation can be easily determined. SENSIT prints all design sensitivity information, as defined in Eqs. (3) through (11), separately for neutrons and gamma rays, and for each perturbed zone, as well as integrated over all perturbed zones.

C. Vector Cross-Section Sensitivity and Uncertainty Analysis (ITYP = 2)

The term "vector cross-section" has been chosen to identify a multigroup cross-section set which consists of a linear string of numbers with one group-averaged reaction cross-section per group, but no scattering matrix. Existing correlations between two individual vector cross-sections are easily described by a simple two-dimensional correlation matrix. As a consequence, therefore, it is also straightforward to describe correlated cross-section uncertainties of pairs of vector cross-sections by a two-dimensional covariance matrix [5]. For ITYP = 2, SENSIT performs a complete sensitivity and response uncertainty analysis for given sets of vector cross-section pairs $\{Z_1^R\}$ and $\{Z_2^R\}$ with an associated covariance matrix $\text{Cov}(Z_1^R, Z_2^R)$ attached to each pair. As a first step SENSIT calculates the sensitivity profiles p_1^R and p_2^R for each individual vector cross section. Then the covariance matrix $\text{Cov}(Z_1^R, Z_2^R)$ is used to compute the resulting integral response uncertainty due to the correlated cross-section uncertainties of this pair of vector cross sections according to [6]

$$\text{Var}(I_{\phi}) = \sum_{k=1}^{16M1} \sum_{l=1}^{16M1} p_1^R \cdot p_2^R \cdot \text{Cov}(Z_1^R, Z_2^R). \quad (12)$$

Both, the variance $\text{Var}(I_{\phi})$ as well as the relative standard deviation

$$\frac{\delta I}{I} = \sqrt{\frac{\text{Var}(I_{\phi})}{I^2}}, \quad (13)$$

are printed by SENSIT for each vector cross-section pair.

D. SED Sensitivity and Uncertainty Analysis (ITYP = 3)

It has only recently been recognized [9] that sensitivity profiles for secondary energy and angular distributions are obtained as adjoints of the standard sensitivity profiles, i.e., from the differential form of the adjoint difference (AD) formulation. For ITYP = 3, SENSIT computes and prints the double-differential and single-differential sensitivity profiles for secondary energy distributions (SED's) and performs also an SED uncertainty analysis based on the hot/cold concept of integral SED uncertainties [10].

As shown in Ref. [9], a double-differential SED sensitivity profile is described by the differential form of the gain term in the AD-formulation:

$$p_{SED}^{g',g} = \left\{ \sum_{l=0}^{LMAX} z_{s,l}^{g',g} \cdot \psi_l^{g',g} \right\} / I_0 \cdot \Delta u^{g'} \cdot \Delta u^g \quad (14)$$

This double-differential SED sensitivity profile quantifies the sensitivity of the integral response I_0 to the scattering matrix element $z_{s,l}^{g',g}$. Therefore, $p_{SED}^{g',g}$ is a pure gain term for the sensitivity gain due to the transfer of neutrons from the incident energy group g' to the final energy group g .

In order to perform an SED uncertainty analysis based on the hot/cold concept introduced in Ref. [10], it is required to specify the median energy group of the SED for each incident neutron energy group, $GMED(g')$, as well as the associated integral SED uncertainty (spectral shape uncertainty parameter), $F_{SED}(g')$, for each SED with incident energy group g' . $GMED(g')$ and $F_{SED}(g')$ are expected input arrays in SENSIT if ITYP = 3. Hot and cold integral SED sensitivity coefficients, $S_{HOT}(g')$ and $S_{COLD}(g')$, are then computed by SENSIT according to [10]:

$$S_{HOT}(g') = \Delta u^{g'} \cdot \sum_{g=GMED(g')}^{GMED(g')} p_{SED}^{g',g} \cdot \Delta u^g \quad (15)$$

$$S_{COLD}(g') = \Delta u^{g'} \cdot \sum_{g=GMED(g')+1}^{LGM1} p_{SED}^{g',g} \cdot \Delta u^g \quad (16)$$

From these two components of an integral SED sensitivity, SENSIT obtains the net integral SED sensitivity coefficient

$$S(g') = S_{HOT}(g') - S_{COLD}(g') \quad (17)$$

which quantifies how much more sensitive the integral response I_0 is to the hot component of the SED at incident energy group g' than to its cold component. The simplest possible response uncertainty estimate due to estimated SED uncertainties is then obtained from [10]

$$\left(\frac{\delta I}{I} \right)_{SED} = \sum_{g'=1}^{LGM1} |S(g')| \cdot F_{SED}(g') \quad (18)$$

Values for the SED sensitivity profile, as defined in Eq. (14), all integral SED sensitivity coefficients, Eqs. (15) through (17), and the estimated response uncertainty due to all integral SED uncertainties according to Eq. (18), are printed by SENSIT for each set of material cross sections and associated integral SED uncertainties.

4. Input Formats.

SENSIT uses the angular flux output from one-dimensional discrete-ordinates codes as input files. Slab, spherical and one-dimensional cylindrical geometries are allowed. An input parameter ITAPE allows to read angular forward- and adjoint-flux tapes in two different formats. ITAPE = 1 is the preferred option to read the standardized CCCF-flux format which is defined precisely [11] and is recommended by the Committee on Computer Code Coordination as a code and computer independent standard interface format. The LASL code ONETRAN [12], e.g., generates a CCCF-formatted angular flux tape on TAPE11 if both control integers IFO and IANG are set to 1. If ITAPE = 0, SENSIT reads the angular flux tapes as generated by the ORNL code ANISN [13] or the older LASL code DTF [14].

Three options are built into SENSIT to read standard neutron (or coupled neutron/gamma-ray multi-group cross-section sets: first, LASL format cross sections from cards; second, LASL format cross sections from tape; and third, limited FIDO (ORNL) format cross sections from cards. The general structure of all transport cross-section tables is as described in the transport code literature; e.g., the ONETRAN [12] or ANISN manual [13]. The LASL format is simply a string of 6E12.5 formatted numbers, while the FIDO format allows certain abbreviations for strings of zeroes, etc. For covariance data input a convenient ENDF-like input format is adopted which is identical to the output format from the cross-section processing code system NJOY [15].

5. Data Management and Storage Requirements:

SENSIT uses one-, two-, and three-dimensional arrays to manage the large amount of numerical data involved in its execution. Core storage is reserved for a particular dimensioned array only during the time the corresponding data are required to be in-core; at other times, the space is made available for the storage of other data. In order to alleviate bookkeeping chores associated with such dynamic storage allocation techniques, Argonne National Laboratory developed a collection of subroutines, called the BPOINTR package [16,17], which is incorporated in SENSIT. The user needs to know nothing about the BPOINTR routines themselves, only that they require two large blocks of workspace called "containers" for data storage during execution of a job. The container sizes are set in the main program by four FORTRAN statements as explained in Ref. [2], and the choice of sizes is problem dependent. The first container, the FCM (fast-core memory) or SCM (small-core memory) container, is in the CDC-7600's fast memory. The second, the ECM (extended-core-memory) or LCM (large-core memory) container, is in the slower memory banks of the CDC-7600. On IBM machines, both containers are in fast memory [16,17].

6. Machine Requirements and Restrictions

Due to the variable dimensioning as described above, large flexibility exists to adjust the storage requirements for a specific problem to the available machine core. On a CDC-7600 all of the 8 sample problems and the realistic applications described in Ref. [3] could be executed within a maximum of 24000 words of fast (SCM) core and 80000 words of extended-core (ECM) memory.

7. Running Time

A typical execution time on the CDC-7600 for a standard cross-section sensitivity analysis, together with an SED uncertainty analysis is about 4 seconds CPU (central processor units) time. Here a coupled neutron/gamma group structure of 30×12 groups, P_0 cross-sections, and 137 spatial intervals was used. A typical vector cross-section sensitivity and uncertainty analysis with 30×30 covariance matrices requires about 2 seconds of CPU time per case.

8. Material Available:

The SENSIT code package is available in a CDC as well as an IBM version and is distributed through the RSIC/EPIC code center for the U.S. and the ESIS code center for Europe. The package contains the FORTRAN source code together with complete input and output files for 8 sample problems.

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